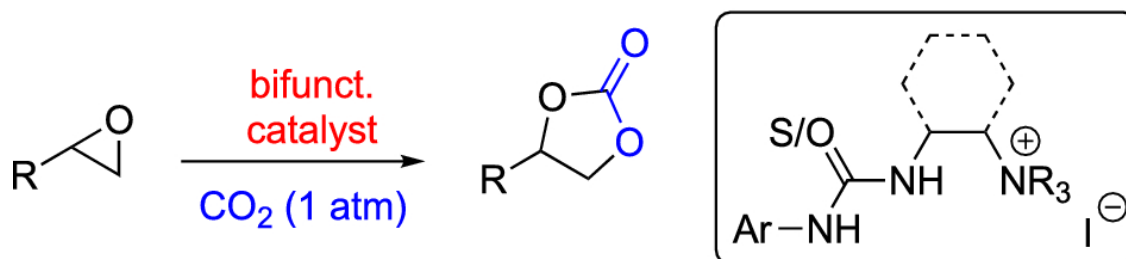


(Thio)urea Containing Quaternary Ammonium Salts for the CO₂-Fixation with Epoxides

Johannes Schörgenhumer, Maximilian Tiffner, and Mario Waser

Institute of Organic Chemistry, Johannes Kepler University Linz, 4040 Linz, Austria

The cycloaddition of CO₂ to epoxides to obtain cyclic carbonates is of broad interest from a synthetic and environmental point of view and the development of suitable catalyst systems for this transformation is an ongoing challenge. In many cases, the approaches rely on the use of metal catalysts and the application of harsh reaction conditions, such as high pressures of CO₂ or elevated reaction temperatures. Herewith, our group's contribution to the topic shall be presented: In line with our long-standing tradition of organocatalysis, charge-containing thiourea catalysts were used to effectively activate epoxides for the cycloaddition. Using only 0.5 - 1 mol% of those organic bifunctional catalysts, the cyclic carbonates were obtained in high yields by the fixation of CO₂ under mild, metal-free and operationally simple conditions (no solvent, 60 °C, atmospheric CO₂ pressure). Complementing these unique results, extensive DFT investigations were carried out and granted an interesting insight into the reaction mechanism [1, 2].



[1] J. Schörgenhumer, M. Tiffner, M. Waser, *Monatsh. Chem.*, **2019**, *accepted* (DOI: 10.1007/s00706-019-02391-w);

[2] Y. Fan, M. Tiffner, J. Schörgenhumer, R. Robiette, M. Waser, S. R. Kass, *J. Org. Chem.*, **2018**, *83*, 9991-10000.